

A vectorial form of the Schrödinger equation

Guy Barrand*

LAL, Univ Paris-Sud, IN2P3/CNRS, Orsay, France

June 2014

Abstract

We rewrite the time dependent Schrödinger equation by using only three dimensional vector algebra and by avoiding to introduce any complex numbers. We show that this equation leads to the same conclusions than the “complex version” concerning the hydrogen atom and the harmonic oscillator. We show also that this equation can be written as a Maxwell-Ampère equation.

Keywords: Schrödinger, Maxwell, Ampère, vector, geometry.

PACS numbers: 03.65.Ta, 03.65.Ca

1 The vectorial Schrödinger equation

Instead of writing the time dependent Schrödinger equation as

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2\mu} \Delta \psi + V \psi$$

we write it:

$$\hbar \frac{\partial}{\partial t} \{ \vec{\psi} \wedge \vec{\iota} \} = -\frac{\hbar^2}{2\mu} \Delta \vec{\psi} + V \vec{\psi} \quad (1)$$

with $\vec{\iota}(t, \vec{x})$ being a real unit three dimensional space direction ($\vec{\iota} \cdot \vec{\iota} = 1$), $\vec{\psi}(t, \vec{x})$ being a three dimensional real vector field and \wedge being the vector wedge product. This equation does not contain complex numbers.

*barrand@lal.in2p3.fr

2 The time independent vectorial Schrödinger equation

By taking a fix \vec{t} we can recover the time independent Schrödinger equation with a $\vec{\psi}(t, \vec{x})$ real vector field of the form:

$$\vec{\psi}(t, \vec{x}) = \exp\left(-\frac{Et}{\hbar} \vec{t} \cdot \vec{\omega}\right) \vec{\rho}(\vec{x}) \quad (2)$$

with $\vec{\rho}(\vec{x})$ being a real vector field orthogonal to \vec{t}

$$\vec{t} \cdot \vec{\rho}(\vec{x}) = 0$$

and $\vec{\omega}$ being the three matrices:

$$(\omega_x)_k^j = \epsilon_{1jk} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}$$

$$(\omega_y)_k^j = \epsilon_{2jk} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

$$(\omega_z)_k^j = \epsilon_{3jk} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

with $j, k, l = 1, 2, 3$ and ϵ_{jkl} being the Levi-Civita symbol. With all indices (2) looks:

$$\psi^j = \left[\exp\left(-\frac{Et}{\hbar} \iota^l \omega^l\right) \right]_k^j \rho^k$$

$\vec{\omega}$ is similar to $\vec{\sigma}$ formed with the three Pauli matrices, and we have for example:

$$((\vec{v} \cdot \vec{\omega})(\vec{w} \cdot \vec{\omega}))_k^j = w^j v^k - (\vec{v} \cdot \vec{w}) \delta_k^j$$

$$(with \vec{\sigma} we have : ((\vec{v} \cdot \vec{\sigma})(\vec{w} \cdot \vec{\sigma}))_k^j = i[(\vec{v} \wedge \vec{w}) \cdot \vec{\sigma}]_k^j + (\vec{v} \cdot \vec{w}) \delta_k^j)$$

As we can write:

$$\frac{\partial}{\partial t} \{ \vec{\psi} \wedge \vec{t} \} = \frac{\partial \vec{\psi}}{\partial t} \wedge \vec{t} = (\vec{t} \cdot \vec{\omega}) \frac{\partial \vec{\psi}}{\partial t}$$

$$(with all indices it looks : \epsilon_{ljk} \frac{\partial \psi^j}{\partial t} \iota^k = \iota^k \epsilon_{klj} \frac{\partial \psi^j}{\partial t} = (\iota^k \omega^k)_j^l \frac{\partial \psi^j}{\partial t})$$

and:

$$\frac{\partial \vec{\psi}}{\partial t} = -\frac{E}{\hbar}(\vec{l} \cdot \vec{\omega})\vec{\psi}$$

Since $\vec{l} \cdot \vec{\psi} = 0$ (because $\vec{l} \cdot \vec{\rho} = 0$) we have:

$$\frac{\partial \vec{\psi}}{\partial t} \wedge \vec{l} = -\frac{E}{\hbar}((\vec{l} \cdot \vec{\omega})(\vec{l} \cdot \vec{\omega}))\vec{\psi} = -\frac{E}{\hbar}(\vec{l}(\vec{l} \cdot \vec{\psi}) - \vec{\psi}) = \frac{E}{\hbar}\vec{\psi}$$

Then our vectorial equation (1) reduces for this particular form (2) of $\vec{\psi}$ to a time independent Schrödinger equation over the vector field $\vec{\rho}(\vec{x})$:

$$E\vec{\rho}(\vec{x}) = -\frac{\hbar^2}{2\mu}\Delta\vec{\rho}(\vec{x}) + V\vec{\rho}(\vec{x})$$

2.1 Recovering the hydrogen atom

To recover the hydrogen atom, we seek a $\vec{\rho}(\vec{x})$ of the form:

$$\vec{\rho}(r, \theta, \phi) = R(r, \theta) \exp(m\phi\vec{l} \cdot \vec{\omega})\vec{\kappa}$$

with $\vec{\kappa}$ being a fix unit vector orthogonal to \vec{l} and m being an integer number in order to recover the same $\vec{\rho}$ after a 2π rotation around \vec{l} ($\vec{\rho}(r, \theta, \phi + 2\pi) = \vec{\rho}(r, \theta, \phi)$). As we have:

$$\frac{\partial^2 \vec{\rho}}{\partial^2 \phi} = -m^2 \vec{\rho}$$

we can proceed as usual by using the Laplacian in spherical coordinates:

$$\Delta\vec{\rho} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial \vec{\rho}}{\partial r}) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \frac{\partial \vec{\rho}}{\partial \theta}) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \vec{\rho}}{\partial^2 \phi}$$

leading on $R(r, \theta)$ only to:

$$\Delta R = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial R}{\partial r}) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \frac{\partial R}{\partial \theta}) - m^2 \frac{R}{r^2 \sin^2 \theta}$$

and then to the traditional "r, θ " Schrodinger equation:

$$-\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial R}{\partial r}) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \frac{\partial R}{\partial \theta}) - m^2 \frac{R}{r^2 \sin^2 \theta} \right] + VR = ER$$

With a Coulombian potential:

$$V = -\frac{e^2}{r}$$

we can proceed as usual; if E is quantised with:

$$E_n = \frac{E_0}{n^2}$$

we have the solutions:

$$R_{nlm}(r, \theta) = \rho_{nl}(r)Y_{lm}(\theta)$$

$$\vec{\rho}_{nlm}(r, \theta, \phi) = \rho_{nl}(r)Y_{lm}(\theta) \exp(m\phi\vec{t} \cdot \vec{\omega})\vec{\kappa}$$

and the real vector field solutions :

$$\vec{\psi}_{nlm\vec{\kappa}}(t, r, \theta, \phi) = \rho_{nl}(r)Y_{lm}(\theta) \exp(-\frac{E_n t}{\hbar}\vec{t} \cdot \vec{\omega}) \exp(m\phi\vec{t} \cdot \vec{\omega})\vec{\kappa}$$

2.2 3D harmonic oscillator

In the same way, with the potential:

$$V = \frac{1}{2}\mu\omega^2 r^2$$

and the energy quantised as:

$$E_{kl} = \hbar\omega(2k + l + \frac{3}{2})$$

we have the real vector field solutions :

$$\vec{\psi}_{klm\vec{\kappa}}(t, r, \theta, \phi) = \rho_{kl}(r)Y_{lm}(\theta) \exp(-\frac{E_{kl} t}{\hbar}\vec{t} \cdot \vec{\omega}) \exp(m\phi\vec{t} \cdot \vec{\omega})\vec{\kappa}$$

3 Vectorial Schrödinger = Maxwell-Ampère

If rewriting (1) as:

$$\partial_0\{\vec{\psi} \wedge \vec{t}\} = -\frac{\xi}{2}\Delta\vec{\psi} + \mathcal{V}\vec{\psi} \quad (3)$$

with dimensions being $[\xi = \frac{\hbar}{\mu c}] = L$, $[\mathcal{V}] = 1/L$ and $\partial_0 = \frac{\partial}{c\partial t}$. By using:

$$\text{rot rot } \vec{\psi} = \text{grad div } \vec{\psi} - \Delta\vec{\psi}$$

we can write:

$$\text{rot}\{\frac{\xi}{2}\text{rot } \vec{\psi}\} = \partial_0\{\vec{\psi} \wedge \vec{t}\} + \frac{\xi}{2}\text{grad div } \vec{\psi} - \mathcal{V}\vec{\psi} \quad (4)$$

By defining $\vec{H}, \vec{D}, \vec{j}$ as:

$$\vec{H} = \chi\frac{\xi}{2}\text{rot } \vec{\psi} \quad (5)$$

$$\vec{D} = \chi\vec{\psi} \wedge \vec{t}$$

$$\frac{\vec{j}}{c} = \chi\{\frac{\xi}{2}\text{grad div } \vec{\psi} - \mathcal{V}\vec{\psi}\}$$

(χ being a constant), we can write (4) as the Maxwell-Ampère equation:

$$\text{rot } \vec{H} = \frac{\partial \vec{D}}{c\partial t} + \frac{\vec{j}}{c} \quad (6)$$

3.1 Other Maxwell equations

The form of (5) strongly suggests to introduce \vec{A}, \vec{B} as:

$$\begin{aligned}\vec{A} &= \mu_0 \chi \frac{\xi}{2} \vec{\psi} \\ \vec{B} &= \mu_0 \vec{H} = \text{rot } \vec{A}\end{aligned}\tag{7}$$

and then U, \vec{E} as:

$$\vec{E} = -\overrightarrow{\text{grad}} U - \partial_0 \vec{A}$$

which, by construction, leads directly to the Maxwell-Faraday equation:

$$\text{rot } \vec{E} = -\frac{\partial \vec{B}}{c \partial t}$$

and the Maxwell-Thomson equation:

$$\text{div } \vec{B} = 0$$

By defining ρ as:

$$\rho = \chi \text{div} \{ \vec{\psi} \wedge \vec{\iota} \}$$

we have, by construction, the Maxwell-Gauss equation:

$$\text{div } \vec{D} = \rho$$

To be complete, we introduce the usual \vec{M}, \vec{P} vectors:

$$\vec{H} = \frac{\vec{B}}{\mu_0} - \vec{M}$$

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P}$$

We see that (7) induces $\vec{M} = 0$ and that U, \vec{P} are related to $\vec{\psi}, \vec{\iota}$ with:

$$-\epsilon_0 \overrightarrow{\text{grad}} U + \vec{P} = \chi \{ \vec{\psi} \wedge \vec{\iota} + \epsilon_0 \mu_0 \frac{\xi}{2} \partial_0 \vec{\psi} \}$$

3.2 Dimensional analysis

About dimensions, we have arranged to have:

$$[\vec{D}] = [\vec{H}], [\vec{E}] = [\vec{B}] \Rightarrow [\epsilon_0 \mu_0] = 1$$

By choosing the χ constant to be of dimension:

$$[\chi] = \sqrt{\text{energy}[\epsilon_0]}$$

and wanting to have the usual:

$$[\vec{D}] = [\vec{H}] = \sqrt{\frac{energy[\epsilon_0]}{volume}} \Leftrightarrow [\vec{E}] = [\vec{B}] = \sqrt{\frac{energy}{volume[\epsilon_0]}}$$

then we get:

$$[\vec{\psi}] = \frac{1}{\sqrt{volume}}$$

which permit to stick to the fact that the integral:

$$\int d^3x \vec{\psi} \cdot \vec{\psi}$$

is without dimension.

4 Currents

In this paper we do not deal explicitly with the interpretation of $\vec{\psi}$ (and $\vec{\iota}$) but as “charge densities” and “currents” often help to shed lights on ideas we may attach to mathematical symbols, we are going to consider this point now.

4.1 from (3)

By taking the dot product of (3) with $\vec{\psi} \wedge \vec{\iota}$, we have:

$$\partial_0 \{ (\vec{\psi} \wedge \vec{\iota})^2 \} + \xi (\vec{\psi} \wedge \vec{\iota}) \cdot \Delta \vec{\psi} = 0 \quad (8)$$

$$\Leftrightarrow \partial_0 \{ \vec{\psi} \cdot \vec{\psi} - (\vec{\psi} \cdot \vec{\iota})^2 \} + \xi (\vec{\psi} \wedge \vec{\iota}) \cdot \Delta \vec{\psi} = 0 \quad (9)$$

With a constant $\vec{\iota}$, by applying (8) on a (still real) $\vec{\psi}$ of the form:

$$\vec{\psi}(t, \vec{x}) = \exp\{S(t, \vec{x})\vec{\iota} \cdot \vec{\omega}\} \vec{R}(t, \vec{x}) \quad (10)$$

some rather simple algebraic manipulations show that we have:

$$\partial_0 \{ \vec{\psi} \cdot \vec{\psi} - (\vec{\psi} \cdot \vec{\iota})^2 \} + \xi \partial_k \{ \{ \vec{\psi} \cdot \vec{\psi} - (\vec{\psi} \cdot \vec{\iota})^2 \} \partial_k S \} = -\xi (\vec{\psi} \wedge \vec{\iota}) \cdot \exp\{S\vec{\iota} \cdot \vec{\omega}\} \Delta \vec{R}$$

which is a continuity equation that we rewrite:

$$\partial_0 \mathcal{P} + \xi \vec{\partial}(\mathcal{P} \vec{\partial} S) = -\xi (\vec{\psi} \wedge \vec{\iota}) \cdot \exp\{S\vec{\iota} \cdot \vec{\omega}\} \Delta \vec{R} \quad (11)$$

with \mathcal{P} being then the positive density:

$$\mathcal{P} = \vec{\psi} \cdot \vec{\psi} - (\vec{\psi} \cdot \vec{\iota})^2 = (\vec{\psi} \wedge \vec{\iota})^2$$

If imposing:

$$\vec{R}(t, \vec{x}) = R(t, \vec{x})\vec{\kappa} \quad (12)$$

with $\vec{\kappa}$ being a fix unit vector orthogonal to \vec{l} , then the right side term of (11) disappears and remains:

$$\frac{\partial(R^2)}{c\partial t} + \xi\vec{\partial}(R^2\vec{\partial}S) = 0$$

which is the usual “probability continuity” equation found in quantum mechanics text books. It is interesting to note that in the case of the more general “oriented” $\vec{\psi}$ of the form (10) the equation (11) does not reduce to this last equation, but have anyway a positive density \mathcal{P} which does not reduce to $\vec{\psi} \cdot \vec{\psi}$.

4.2 from Maxwell

By taking the divergence of (6), we have the conservation equation:

$$\frac{\partial\rho}{\partial t} + \text{div } \vec{j} = 0 \quad (13)$$

but with a ρ being not compelled to be positive. Maxwell equations lead also to a continuity equation on a positive energy density:

$$\partial_0\mathcal{W} + \text{div } \vec{\mathcal{S}} = -\vec{E} \cdot \left\{ \partial_0\vec{P} + \text{rot } \vec{M} + \frac{\vec{j}}{c} \right\} \quad (14)$$

with \mathcal{W} and $\vec{\mathcal{S}}$ (Poynting vector) being:

$$\mathcal{W} = \frac{1}{2} \left\{ \epsilon_0 \vec{E}^2 + \frac{\vec{B}^2}{\mu_0} \right\}$$

$$\vec{\mathcal{S}} = \frac{1}{\mu_0} \vec{E} \wedge \vec{B}$$

Since we have:

$$\frac{\vec{D}^2}{\epsilon_0} = \frac{\chi^2}{\epsilon_0} \mathcal{P} = \epsilon_0 \vec{E}^2 + \dots$$

(11) is contained in (14) but does not reduce to it. (If attempting to interpret things, we may say that the quantum probability density \mathcal{P} is contained, related to a Maxwellian energy!)

5 $\vec{l}(t, \vec{x})$

The fact that we can write $\vec{l}(t, \vec{x})$, which makes no sense in case of using complex numbers (we can't do $i(t, \vec{x})$), introduces new modelling degrees of freedom which are not explored

in this paper; but one idea could be that the \vec{l} field be used as an ingredient for a “collapse mechanism” to explain why a system “fixes” to an eigen-vector-field $\vec{\psi}_n$ during a measurement or interaction. For the pleasure, we write again (1) with all variables:

$$\hbar \frac{\partial}{\partial t} \{ \vec{\psi}(t, \vec{x}) \wedge \vec{l}(t, \vec{x}) \} = - \frac{\hbar^2}{2\mu} \Delta \vec{\psi}(t, \vec{x}) + V(t, \vec{x}) \vec{\psi}(t, \vec{x}) \quad (15)$$

6 Conclusions

The equation (1) without complex numbers is equivalent to the Schrödinger one and it is remarkable that it leads to Maxwell equations. Being able to extend “ i ” to a field $\vec{l}(t, \vec{x})$ leading to (1) or (15) opens modelling possibilities not explored in this paper. The i introduced by E.Schrödinger in 1925 in his equation had been the startup in microphysics of an algebraic inflation that we find highly non intuitive. (Would you claim to have a full intuitive understanding of all symbols of a SUSY Lagrangian made with non commuting numbers? For our point of view about quantum mechanics interpretations see [4]). By avoiding complex numbers in the grounding Schrödinger equation and using instead common vector geometry, we hope to restore a more close relationship of intuition with microphysics. But we have made only “half the way” since we do not come yet with an interpretation of the $\vec{\psi}$ field which stay unveiled. In particular we do not say if $\vec{\psi}$ is ontic or epistemic, but three dimensional vector fields as $\vec{\psi}, \vec{l}$ would tend to an ontic field interpretation.

References

- [1] Erwin Schrödinger *An Undulatory Theory of the Mechanics of Atoms and Molecules*, Phys. Rev., vol. 28, no 6, december 1926, p. 1049-1070
- [2] L.Landau, E.Lifchitz *Mécanique Quantique* (Éditions MIR, Moscou)
- [3] L.Landau, E.Lifchitz *Théorie des Champs* (Éditions MIR, Moscou)
- [4] G.Barrand *Is Nature OO?* arXiv:1108.0014.